Specific analysis of the total energy separates the needs for electricity and heating of processes and process streams. The design-based methodology yielded an intermediate value for heating, 12,559 MJ/1,000 kg ammonia (databases range, 6,094-14,696 MJ/1,000 kg ammonia). However, we have a higher electricity estimate. Since electricity is only about 4% of the total energy, the influence of the overprediction is of less consequence to total energy requirements.

3 Conclusions

Unfortunately, the substances that are included in the most common LCA databases represent just a part of the raw materials used in chemical and biochemical companies, and it is not easy to obtain the information from the manufacturers due to legal, or intellectual property concerns. Besides, frequently the response time from the manufacturers are extremely long, even longer than the time scope for the study.

Therefore, it is common that the practitioners suffer from incomplete or missing information. This sometimes becomes one of the uncertainty sources in the LCA outcome. Furthermore, it could make LCA practitioners give up the implementation of LCA.

LCI information from the North Carolina State University methodology (ab initio calculations) suggested in this paper is useful to LCA practitioners when the information in both foreground and background system is not available. It can reduce the uncertainty associated with the data gaps.

In general, it was found that the results obtained with the proposed methodology are consistent with the existing information. In the case study for ammonia production, the apparent differences found between this methodology and other databases are mainly due to the degree of transparency of the information presented. Another source of differences is that this methodology includes additional issues that normally are not measured (e.g. fugitive emissions), and therefore these are not likely to be reported in other databases.

The design-based approach using repeatable rules provides very comparable LCI values to the industrial measured information when one examines the large parameters, inputs, by-products, CO_2 emissions and specific energy requirements. An industrial verification correction of about 20% in energy led to the closer results from the design-based approach. However, even without this refinement, the major process emissions and inputs were close to field measurements and energy, within 20%. In the large scale use of LCI information for complex studies, such variation is small compared to having to use zero values because data are unavailable.

Like other methodologies, this one has uncertainties. For instance, the uncertainties may be caused by the choice of efficiency of reactor/separation, the efficiency of boiler/heat transfer, or the choice of process types. Sensitivity analysis however, can overcome those uncertainties.

It also needs to be taken into account that the methodology proposed is intended to be a dynamic tool. The "rules of thumb" here proposed are open to change with the current trends of the industrial production processes, the improvements of process operations, and of pollution prevention methods and technologies (e.g. fugitive emissions). Such changes can be done in a very transparent approach for improvement.

Another merit of this methodology is the identification of the key unit within a process. Since this calculation is a microscopic analysis, it is easily to identify a key unit. Therefore, LCI information from this methodology can be used more directly in exploring engineering and chemistry changes to improve manufacturing processes.

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